



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 12:35 PM UTC

PDB ID : 9WU2 / pdb_00009wu2
Title : Crystal structure of cZ22-Fab in complex with left-handed dC(GC)3 DNA
Authors : Lee, C.C.; Hsu, S.F.; Ko, T.P.; Wang, A.H.J.
Deposited on : 2025-09-17
Resolution : 2.35 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

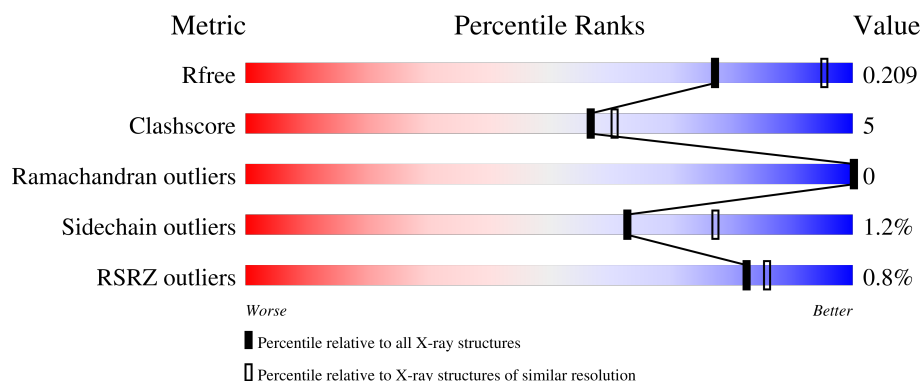
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	236	<div> <div></div> <div>78%</div> <div>12%</div> <div>9%</div> </div>
1	C	236	<div> <div></div> <div>83%</div> <div>8%</div> <div>9%</div> </div>
1	G	236	<div> <div></div> <div>81%</div> <div>10%</div> <div>9%</div> </div>
1	I	236	<div> <div></div> <div>80%</div> <div>10%</div> <div>9%</div> </div>
1	M	236	<div> <div></div> <div>82%</div> <div>8%</div> <div>10%</div> </div>

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Mol	Chain	Length	Quality of chain
1	O	236	 82% 9% 9%
2	B	214	 90% 9%
2	D	214	 93% 7%
2	H	214	 89% 9%
2	J	214	 86% 12%
2	N	214	 91% 8%
2	P	214	 91% 8%
3	E	7	 100%
3	F	7	 100%
3	K	7	 100%
3	L	7	 100%
3	Q	7	 86% 14%
3	R	7	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	C	301	-	X	X	-
4	GOL	G	301	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22292 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called cZ22-Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1624	1026	271	317	10			
1	C	214	Total	C	N	O	S	0	0	0
			1627	1029	272	316	10			
1	G	214	Total	C	N	O	S	0	0	0
			1627	1029	272	316	10			
1	I	214	Total	C	N	O	S	0	0	0
			1627	1029	272	316	10			
1	M	213	Total	C	N	O	S	0	0	0
			1618	1023	270	315	10			
1	O	214	Total	C	N	O	S	0	0	0
			1626	1029	272	315	10			

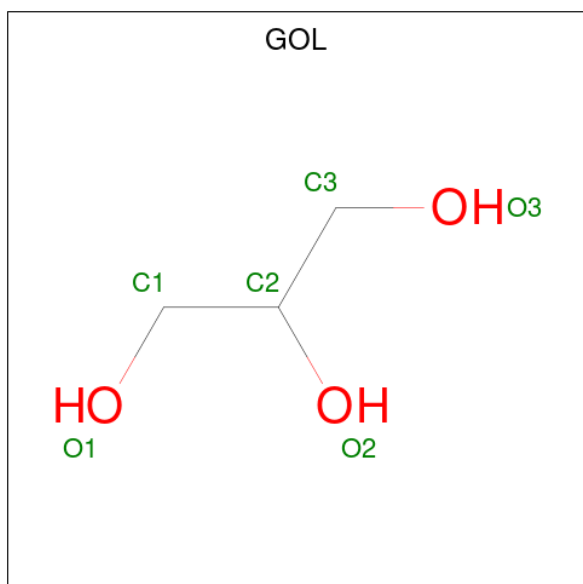
- Molecule 2 is a protein called cZ22-Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	213	Total	C	N	O	S	0	0	0
			1652	1034	274	339	5			
2	D	213	Total	C	N	O	S	0	0	0
			1652	1034	274	339	5			
2	H	213	Total	C	N	O	S	0	0	0
			1652	1034	274	339	5			
2	J	213	Total	C	N	O	S	0	0	0
			1652	1034	274	339	5			
2	N	213	Total	C	N	O	S	0	0	0
			1652	1034	274	339	5			
2	P	213	Total	C	N	O	S	0	0	0
			1652	1034	274	339	5			

- Molecule 3 is a DNA chain called DNA (5'-D(*CP*GP*CP*GP*CP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	7	Total	C	N	O	P	0	1	0
			144	67	27	43	7			
3	F	7	Total	C	N	O	P	0	1	0
			144	67	27	43	7			
3	K	7	Total	C	N	O	P	0	0	0
			139	66	27	40	6			
3	L	7	Total	C	N	O	P	0	1	0
			144	67	27	43	7			
3	Q	7	Total	C	N	O	P	0	0	0
			139	66	27	40	6			
3	R	7	Total	C	N	O	P	0	0	0
			139	66	27	40	6			

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	I	1	Total	C	O	0	0
			6	3	3		
4	M	1	Total	C	O	0	0
			6	3	3		
4	O	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	114	Total	O		0	0
			114	114			
5	B	116	Total	O		0	0
			116	116			
5	C	178	Total	O		0	0
			178	178			
5	D	177	Total	O		0	0
			177	177			
5	E	28	Total	O		0	0
			28	28			
5	F	17	Total	O		0	0
			17	17			
5	G	104	Total	O		0	0
			104	104			
5	H	81	Total	O		0	0
			81	81			
5	I	129	Total	O		0	0
			129	129			
5	J	165	Total	O		0	0
			165	165			
5	K	18	Total	O		0	0
			18	18			
5	L	14	Total	O		0	0
			14	14			
5	M	145	Total	O		0	0
			145	145			
5	N	151	Total	O		0	0
			151	151			
5	O	120	Total	O		0	0
			120	120			
5	P	125	Total	O		0	0
			125	125			

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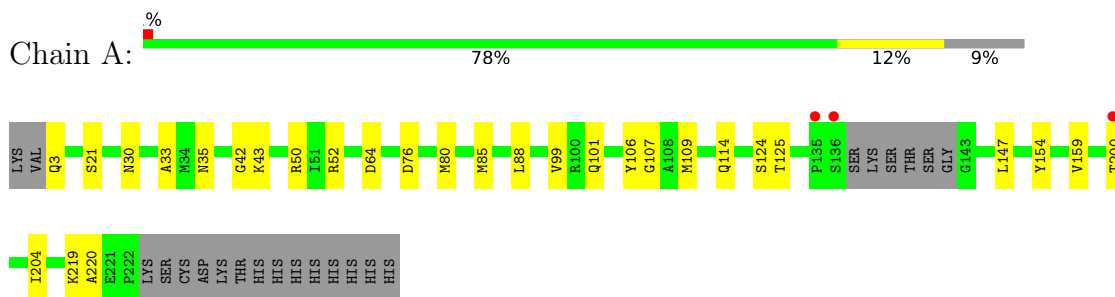
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	Q	28	Total	O	0	0
			28	28		
5	R	24	Total	O	0	0
			24	24		

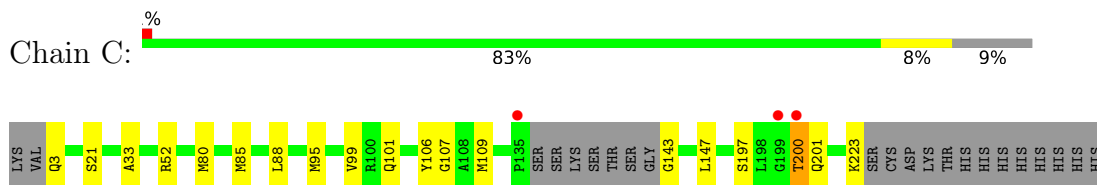
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

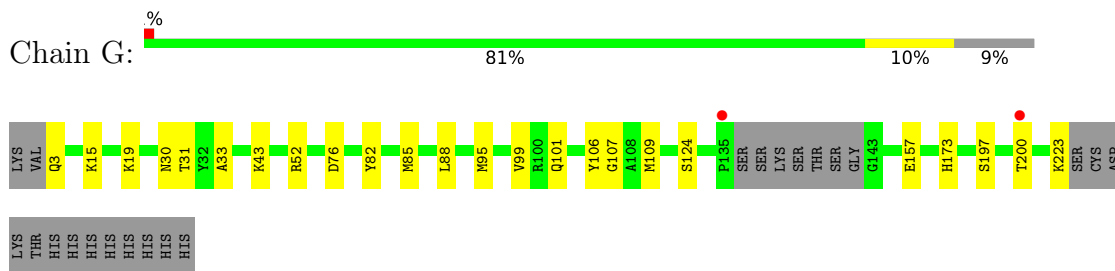
- Molecule 1: cZ22-Fab heavy chain



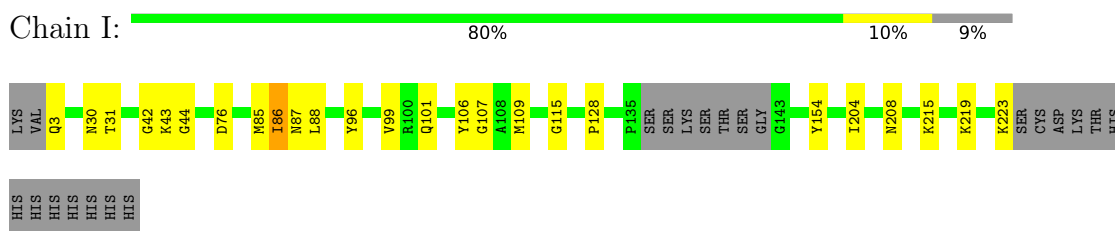
- Molecule 1: cZ22-Fab heavy chain




- Molecule 1: cZ22-Fab heavy chain

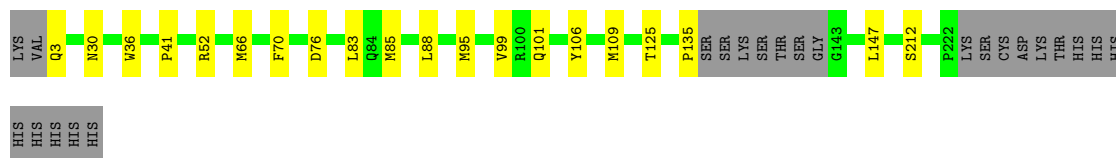


- Molecule 1: cZ22-Fab heavy chain




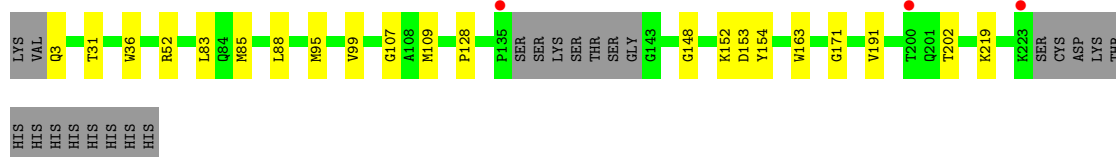
- Molecule 1: cZ22-Fab heavy chain

Chain M:  82% 8% 10%




- Molecule 1: cZ22-Fab heavy chain

Chain O:  82% 9% 9%




- Molecule 2: cZ22-Fab light chain

Chain B:  90% 9%




- Molecule 2: cZ22-Fab light chain

Chain D:  93% 7%




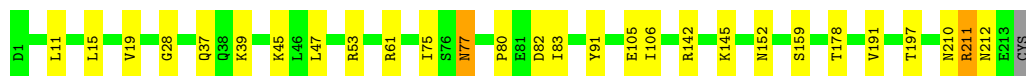
- Molecule 2: cZ22-Fab light chain

Chain H:  89% 9%




- Molecule 2: cZ22-Fab light chain

Chain J:  86% 12%

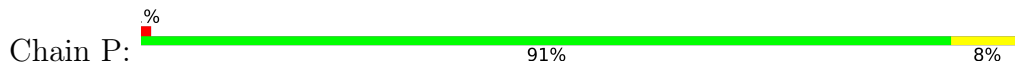


- Molecule 2: cZ22-Fab light chain

Chain N:  91% 8%



- Molecule 2: cZ22-Fab light chain



- Molecule 3: DNA (5'-D(*CP*GP*CP*GP*CP*GP*C)-3')



There are no outlier residues recorded for this chain.

- Molecule 3: DNA (5'-D(*CP*GP*CP*GP*CP*GP*C)-3')



There are no outlier residues recorded for this chain.

- Molecule 3: DNA (5'-D(*CP*GP*CP*GP*CP*GP*C)-3')



There are no outlier residues recorded for this chain.

- Molecule 3: DNA (5'-D(*CP*GP*CP*GP*CP*GP*C)-3')



There are no outlier residues recorded for this chain.

- Molecule 3: DNA (5'-D(*CP*GP*CP*GP*CP*GP*C)-3')



- Molecule 3: DNA (5'-D(*CP*GP*CP*GP*CP*GP*C)-3')



There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	195.57Å 195.57Å 89.39Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	17.92 – 2.35 17.92 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.0 (17.92-2.35) 97.8 (17.92-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.88 (at 2.35Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.169 , 0.210 0.169 , 0.209	Depositor DCC
R_{free} test set	7753 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for -h,-k,l 0.006 for h,-h-k,-l 0.006 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	22292	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PCA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.46	0/1655	0.66	0/2251
1	C	0.53	0/1658	0.69	0/2254
1	G	0.46	0/1658	0.67	0/2254
1	I	0.47	0/1658	0.65	0/2254
1	M	0.50	0/1649	0.65	0/2243
1	O	0.49	0/1657	0.68	0/2253
2	B	0.48	0/1687	0.70	0/2289
2	D	0.57	0/1687	0.68	0/2289
2	H	0.46	0/1687	0.61	0/2289
2	J	0.55	0/1687	0.71	0/2289
2	N	0.50	0/1687	0.68	0/2289
2	P	0.53	0/1687	0.69	0/2289
3	E	0.63	0/180	0.78	0/276
3	F	0.54	0/176	0.73	0/269
3	K	0.59	0/155	0.70	0/237
3	L	0.44	0/176	0.68	0/269
3	Q	0.54	0/155	0.79	0/237
3	R	0.51	0/155	0.79	0/237
All	All	0.50	0/21054	0.68	0/28768

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	J	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	J	211	ARG	Sidechain
2	J	53	ARG	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1624	0	1578	18	0
1	C	1627	0	1586	18	0
1	G	1627	0	1586	20	0
1	I	1627	0	1586	20	0
1	M	1618	0	1573	16	0
1	O	1626	0	1583	14	0
2	B	1652	0	1597	13	0
2	D	1652	0	1597	16	0
2	H	1652	0	1597	14	0
2	J	1652	0	1597	19	0
2	N	1652	0	1597	11	0
2	P	1652	0	1597	11	0
3	E	144	0	74	0	0
3	F	144	0	74	0	0
3	K	139	0	79	0	0
3	L	144	0	74	0	0
3	Q	139	0	79	2	0
3	R	139	0	79	0	0
4	A	6	0	8	3	0
4	C	6	0	8	6	0
4	G	18	0	24	9	0
4	I	6	0	8	1	0
4	M	6	0	8	1	0
4	O	6	0	8	2	0
5	A	114	0	0	1	0
5	B	116	0	0	1	0
5	C	178	0	0	2	0
5	D	177	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	28	0	0	0	0
5	F	17	0	0	0	0
5	G	104	0	0	3	0
5	H	81	0	0	0	0
5	I	129	0	0	1	0
5	J	165	0	0	4	0
5	K	18	0	0	0	0
5	L	14	0	0	0	0
5	M	145	0	0	1	0
5	N	151	0	0	2	0
5	O	120	0	0	0	0
5	P	125	0	0	0	0
5	Q	28	0	0	0	0
5	R	24	0	0	0	0
All	All	22292	0	19597	186	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 186 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:83:ILE:HD11	2:D:106:ILE:HG12	1.38	1.04
1:O:52:ARG:HE	4:O:301:GOL:H31	1.22	1.02
2:P:83:ILE:HD11	2:P:106:ILE:HG12	1.46	0.97
1:G:173:HIS:ND1	4:G:302:GOL:H31	1.87	0.89
1:C:52:ARG:HH21	4:C:301:GOL:H32	1.39	0.84

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	210/236 (89%)	206 (98%)	4 (2%)	0	100	100
1	C	210/236 (89%)	207 (99%)	3 (1%)	0	100	100
1	G	210/236 (89%)	206 (98%)	4 (2%)	0	100	100
1	I	210/236 (89%)	206 (98%)	4 (2%)	0	100	100
1	M	209/236 (89%)	205 (98%)	4 (2%)	0	100	100
1	O	210/236 (89%)	206 (98%)	4 (2%)	0	100	100
2	B	211/214 (99%)	203 (96%)	8 (4%)	0	100	100
2	D	211/214 (99%)	203 (96%)	8 (4%)	0	100	100
2	H	211/214 (99%)	204 (97%)	7 (3%)	0	100	100
2	J	211/214 (99%)	204 (97%)	7 (3%)	0	100	100
2	N	211/214 (99%)	203 (96%)	8 (4%)	0	100	100
2	P	211/214 (99%)	203 (96%)	8 (4%)	0	100	100
All	All	2525/2700 (94%)	2456 (97%)	69 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	178/199 (89%)	174 (98%)	4 (2%)	45	59
1	C	178/199 (89%)	176 (99%)	2 (1%)	65	79
1	G	178/199 (89%)	174 (98%)	4 (2%)	45	59
1	I	178/199 (89%)	176 (99%)	2 (1%)	65	79
1	M	177/199 (89%)	177 (100%)	0	100	100
1	O	177/199 (89%)	176 (99%)	1 (1%)	78	87
2	B	191/192 (100%)	191 (100%)	0	100	100
2	D	191/192 (100%)	191 (100%)	0	100	100
2	H	191/192 (100%)	187 (98%)	4 (2%)	47	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	J	191/192 (100%)	188 (98%)	3 (2%)	55	70
2	N	191/192 (100%)	187 (98%)	4 (2%)	47	61
2	P	191/192 (100%)	189 (99%)	2 (1%)	68	81
All	All	2212/2346 (94%)	2186 (99%)	26 (1%)	63	77

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	31	THR
2	J	152	ASN
2	P	77	ASN
2	J	77	ASN
2	J	212	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
2	J	3	GLN
2	P	212	ASN
1	M	30	ASN
2	P	38	GLN
2	J	210	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PCA	A	3	1	7,8,9	2.08	1 (14%)	9,10,12	1.96	5 (55%)
1	PCA	I	3	1	7,8,9	2.18	1 (14%)	9,10,12	2.54	5 (55%)
1	PCA	M	3	1	7,8,9	2.00	1 (14%)	9,10,12	2.00	5 (55%)
1	PCA	O	3	1	7,8,9	2.10	1 (14%)	9,10,12	2.06	5 (55%)
1	PCA	G	3	1	7,8,9	2.12	1 (14%)	9,10,12	2.16	5 (55%)
1	PCA	C	3	1	7,8,9	2.22	1 (14%)	9,10,12	2.39	5 (55%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PCA	A	3	1	-	0/0/11/13	0/1/1/1
1	PCA	I	3	1	-	0/0/11/13	0/1/1/1
1	PCA	M	3	1	-	0/0/11/13	0/1/1/1
1	PCA	O	3	1	-	0/0/11/13	0/1/1/1
1	PCA	G	3	1	-	0/0/11/13	0/1/1/1
1	PCA	C	3	1	-	0/0/11/13	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	3	PCA	CD-N	5.58	1.48	1.34
1	I	3	PCA	CD-N	5.54	1.48	1.34
1	G	3	PCA	CD-N	5.50	1.48	1.34
1	A	3	PCA	CD-N	5.31	1.47	1.34
1	O	3	PCA	CD-N	5.21	1.47	1.34

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	3	PCA	CB-CA-C	-4.22	106.87	112.66
1	C	3	PCA	CB-CA-C	-3.64	107.66	112.66
1	C	3	PCA	OE-CD-CG	-3.38	120.69	126.72
1	I	3	PCA	OE-CD-CG	-3.29	120.86	126.72
1	I	3	PCA	CA-N-CD	-3.07	103.08	113.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	GOL	C	301	-	5,5,5	1.88	2 (40%)	5,5,5	1.30	1 (20%)
4	GOL	G	301	-	5,5,5	1.58	1 (20%)	5,5,5	0.98	0
4	GOL	G	302	-	5,5,5	1.14	1 (20%)	5,5,5	1.14	1 (20%)
4	GOL	O	301	-	5,5,5	2.05	1 (20%)	5,5,5	0.82	0
4	GOL	I	301	-	5,5,5	1.13	0	5,5,5	1.69	1 (20%)
4	GOL	G	303	-	5,5,5	1.20	0	5,5,5	0.99	0
4	GOL	A	301	-	5,5,5	1.12	0	5,5,5	1.45	1 (20%)
4	GOL	M	301	-	5,5,5	1.50	2 (40%)	5,5,5	0.91	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	C	301	-	-	4/4/4/4	-
4	GOL	G	301	-	-	3/4/4/4	-
4	GOL	G	302	-	-	2/4/4/4	-
4	GOL	O	301	-	-	4/4/4/4	-
4	GOL	I	301	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	G	303	-	-	1/4/4/4	-
4	GOL	A	301	-	-	2/4/4/4	-
4	GOL	M	301	-	-	2/4/4/4	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	O	301	GOL	C1-C2	3.61	1.65	1.51
4	C	301	GOL	C1-C2	3.29	1.64	1.51
4	G	301	GOL	C1-C2	2.79	1.62	1.51
4	C	301	GOL	O1-C1	2.38	1.52	1.42
4	M	301	GOL	C3-C2	2.26	1.60	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	301	GOL	C3-C2-C1	-2.56	102.39	111.80
4	I	301	GOL	C3-C2-C1	-2.47	102.72	111.80
4	A	301	GOL	C3-C2-C1	-2.38	103.05	111.80
4	G	302	GOL	C3-C2-C1	-2.25	103.53	111.80

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	301	GOL	C1-C2-C3-O3
4	C	301	GOL	C1-C2-C3-O3
4	G	301	GOL	O2-C2-C3-O3
4	C	301	GOL	O1-C1-C2-C3
4	G	301	GOL	C1-C2-C3-O3

There are no ring outliers.

7 monomers are involved in 22 short contacts:

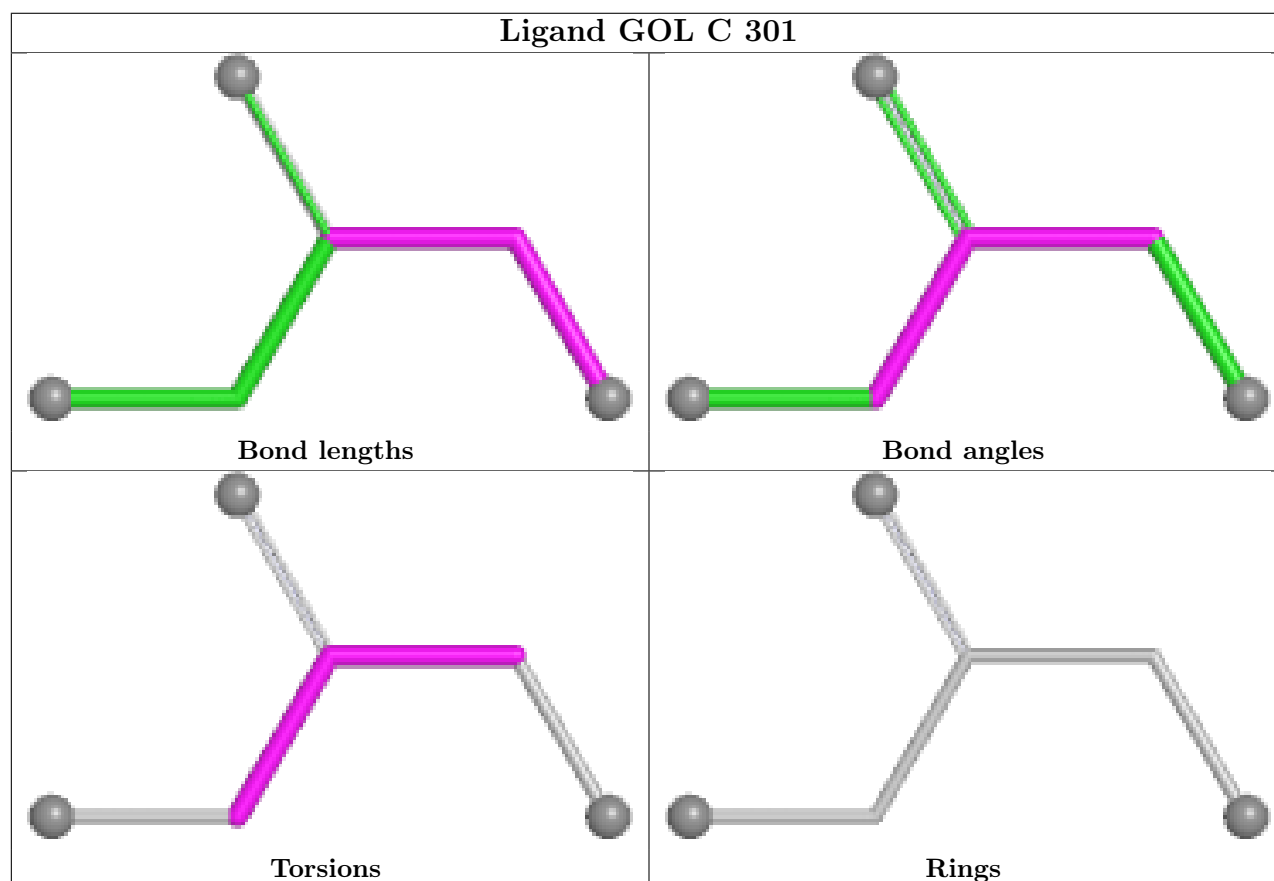
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	301	GOL	6	0
4	G	301	GOL	7	0
4	G	302	GOL	2	0
4	O	301	GOL	2	0
4	I	301	GOL	1	0

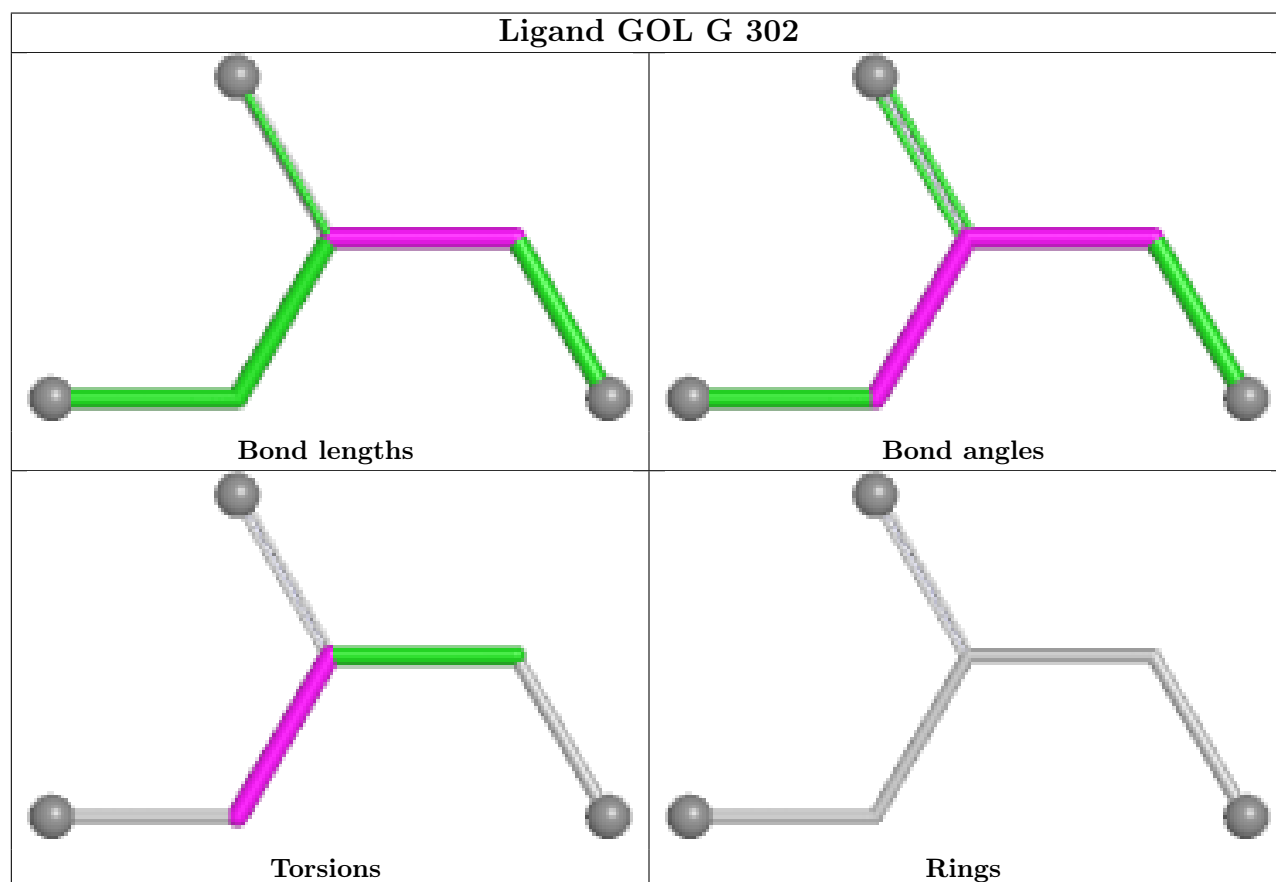
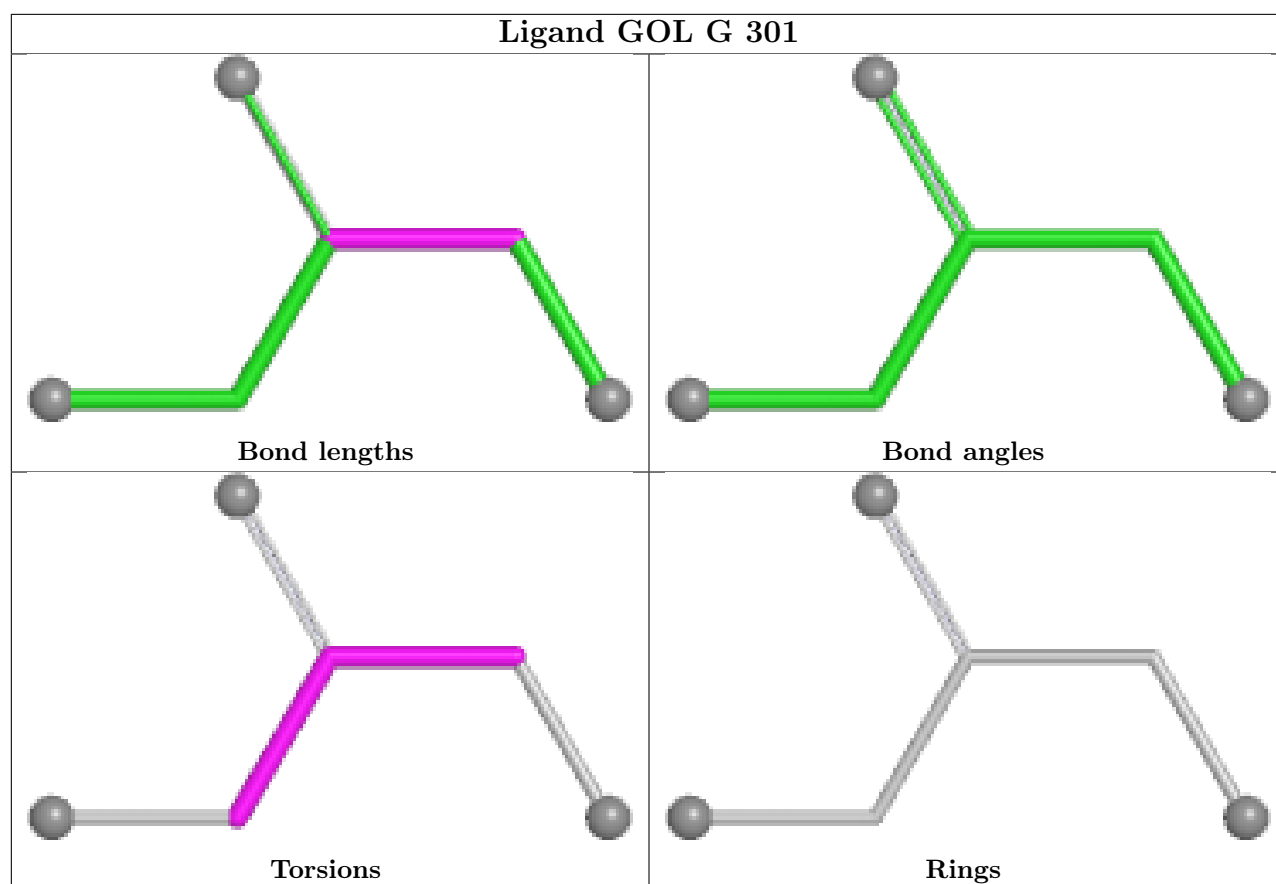
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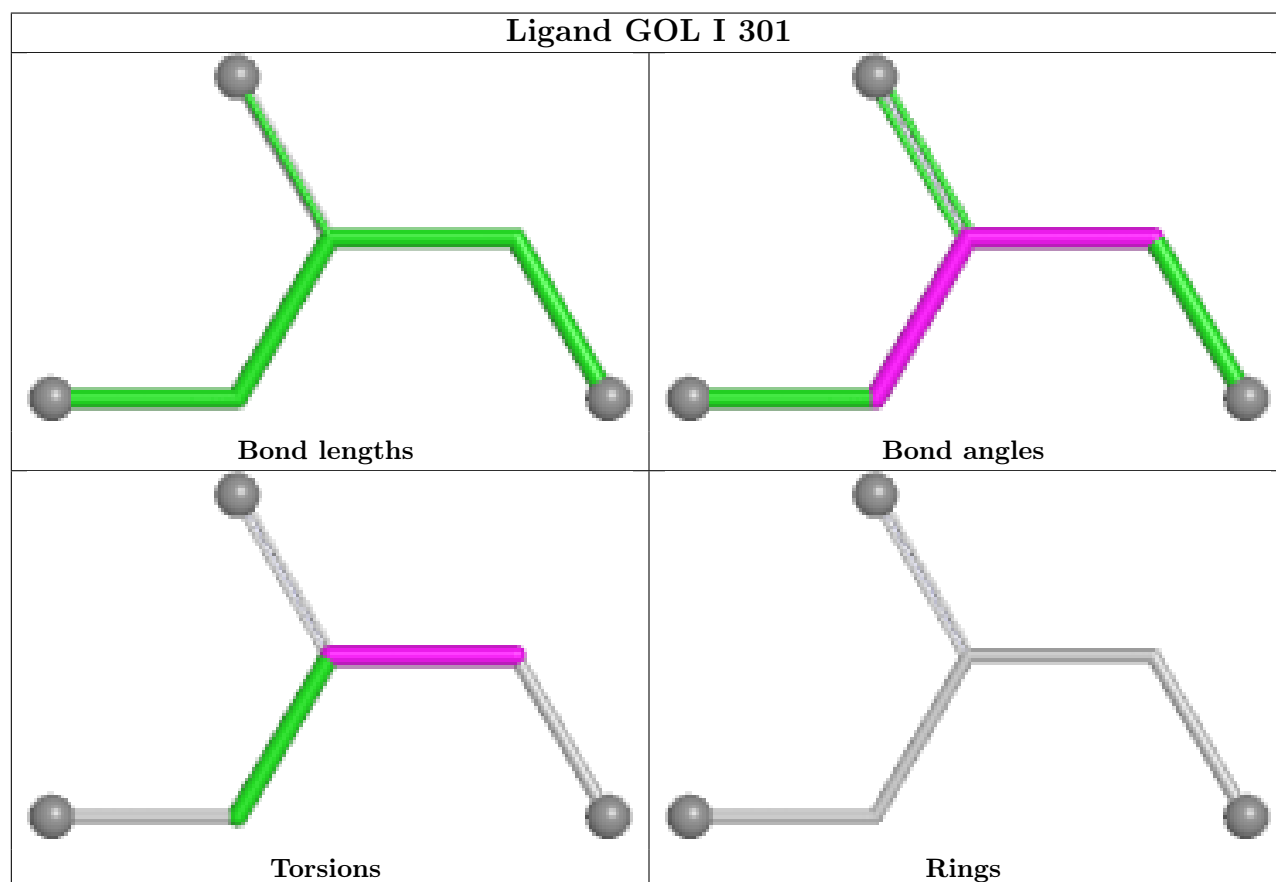
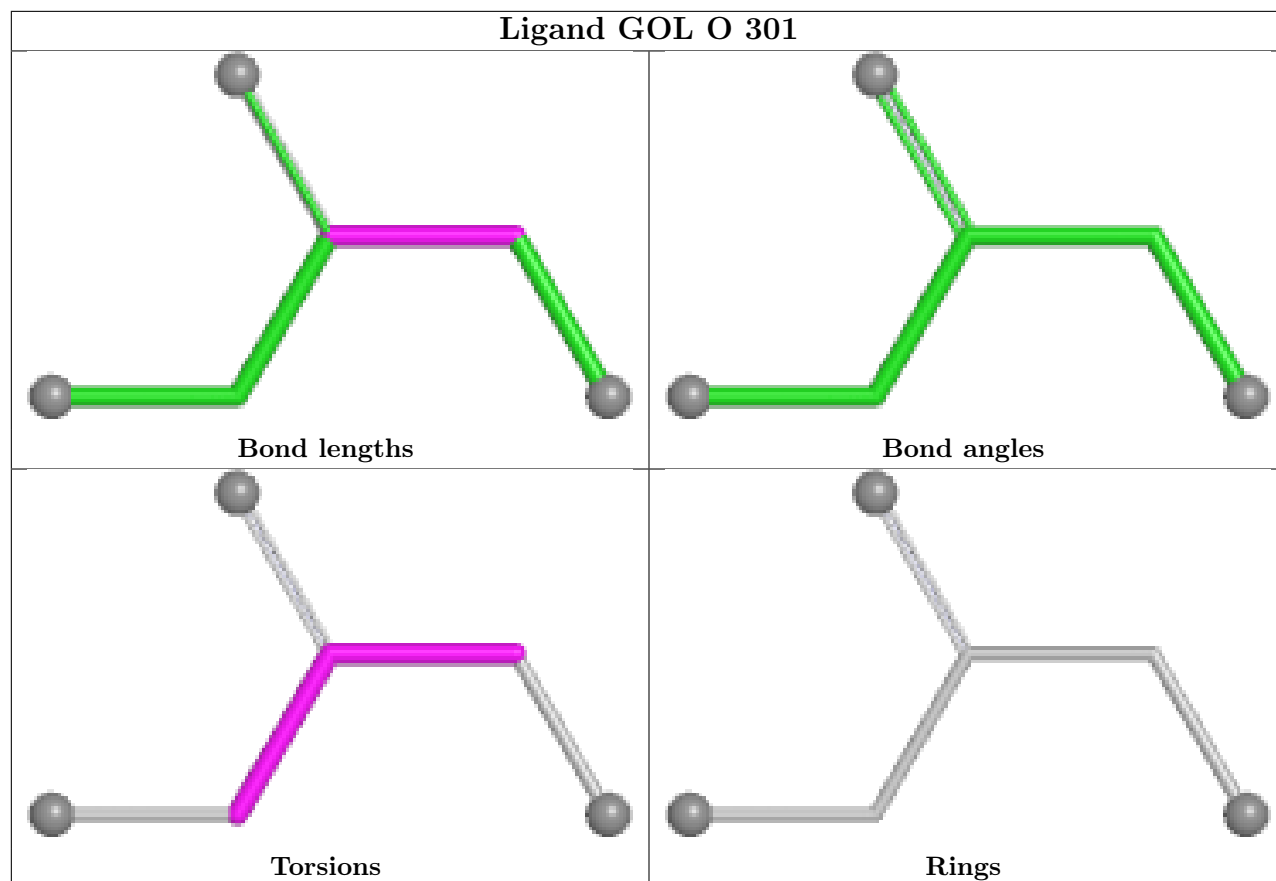
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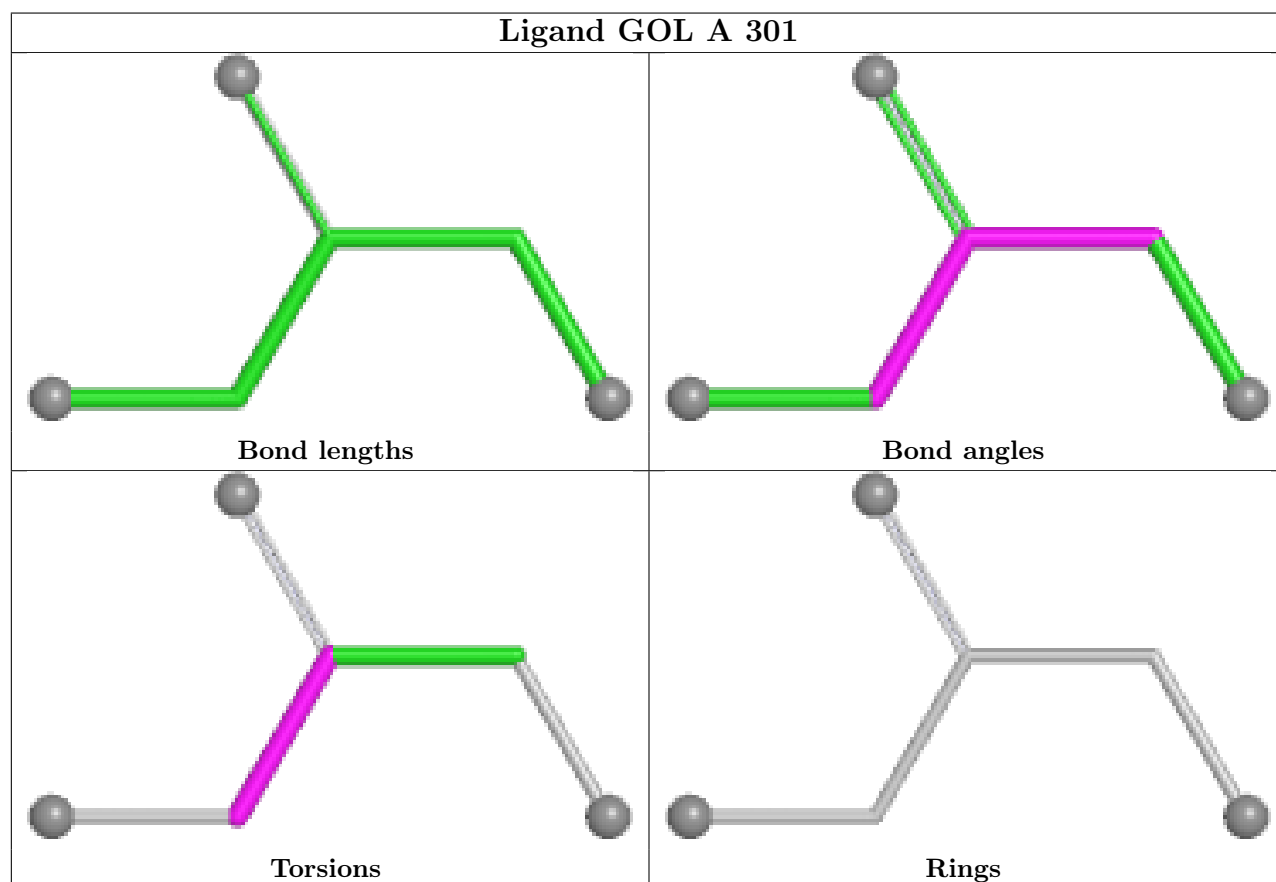
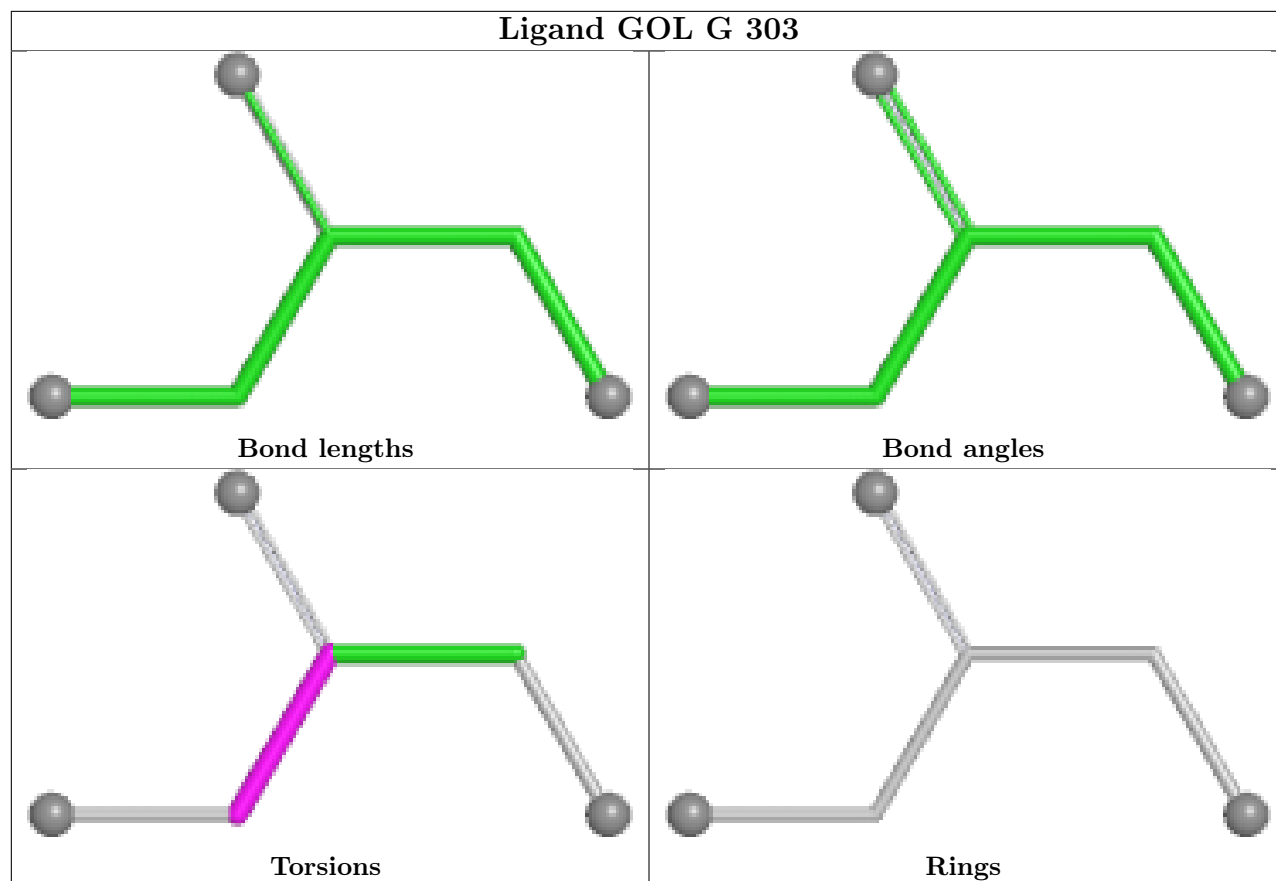
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	301	GOL	3	0
4	M	301	GOL	1	0

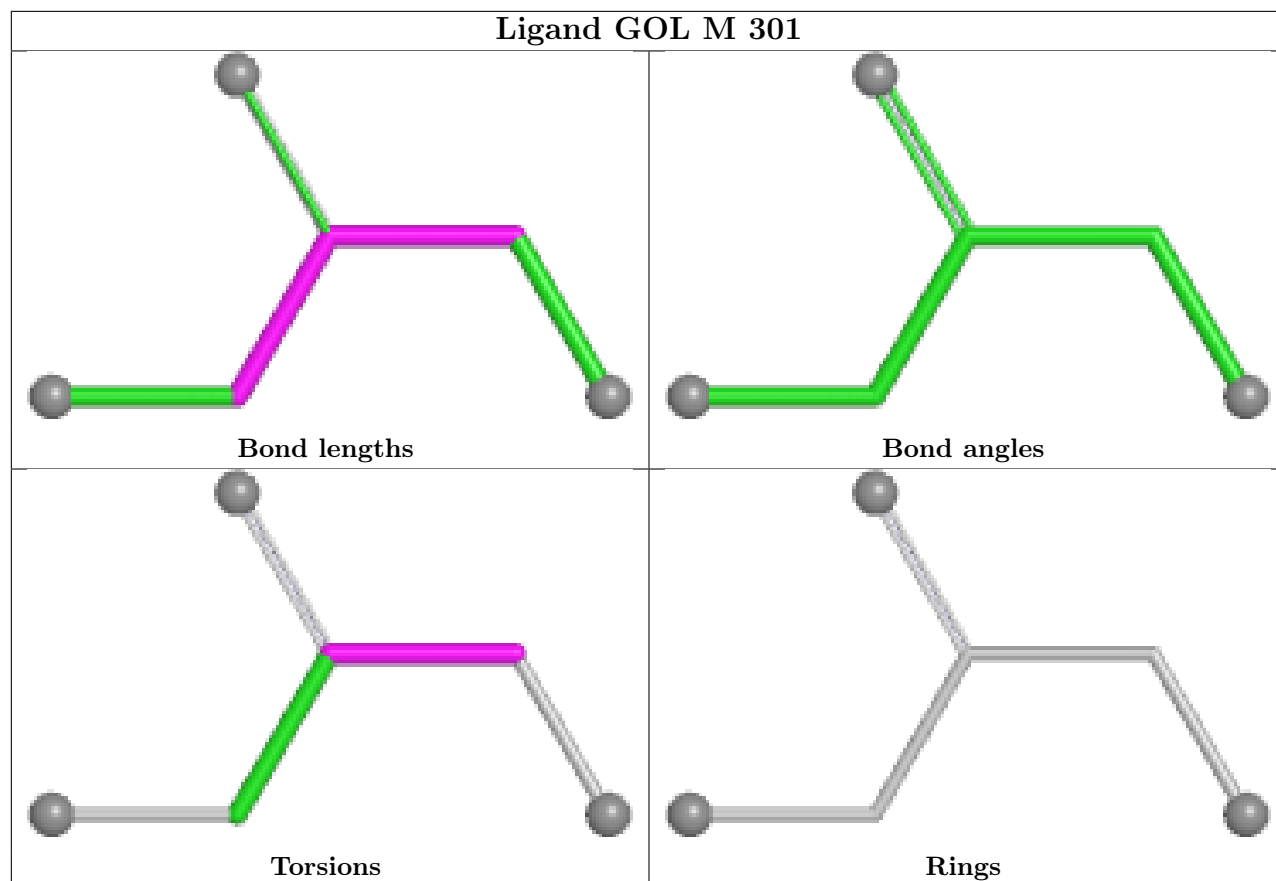
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	213/236 (90%)	-0.35	3 (1%) 73 78	23, 38, 61, 83	0
1	C	213/236 (90%)	-0.53	3 (1%) 73 78	18, 28, 55, 86	0
1	G	213/236 (90%)	-0.22	2 (0%) 81 84	26, 39, 71, 91	0
1	I	213/236 (90%)	-0.36	0 100 100	24, 37, 63, 75	0
1	M	212/236 (89%)	-0.42	0 100 100	20, 35, 56, 78	0
1	O	213/236 (90%)	-0.30	3 (1%) 73 78	22, 37, 65, 86	0
2	B	213/214 (99%)	-0.29	1 (0%) 87 90	24, 38, 63, 116	0
2	D	213/214 (99%)	-0.48	2 (0%) 81 84	19, 32, 52, 116	0
2	H	213/214 (99%)	0.08	3 (1%) 73 78	31, 48, 79, 115	0
2	J	213/214 (99%)	-0.48	0 100 100	20, 33, 52, 91	0
2	N	213/214 (99%)	-0.39	1 (0%) 87 90	20, 34, 58, 109	0
2	P	213/214 (99%)	-0.39	3 (1%) 73 78	23, 37, 55, 109	0
3	E	7/7 (100%)	-1.15	0 100 100	25, 27, 35, 43	1 (14%)
3	F	7/7 (100%)	-0.95	0 100 100	28, 33, 44, 47	1 (14%)
3	K	7/7 (100%)	-1.02	0 100 100	38, 40, 47, 50	0
3	L	7/7 (100%)	-0.76	0 100 100	35, 41, 48, 52	1 (14%)
3	Q	7/7 (100%)	-1.21	0 100 100	29, 31, 41, 46	0
3	R	7/7 (100%)	-0.92	0 100 100	31, 33, 41, 44	0
All	All	2597/2742 (94%)	-0.36	21 (0%) 82 86	18, 36, 63, 116	3 (0%)

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	135	PRO	3.9
1	G	200	THR	3.6
2	H	7	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	200	THR	3.2
1	C	199	GLY	3.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	PCA	I	3	8/9	0.90	0.10	48,52,61,61	0
1	PCA	G	3	8/9	0.92	0.09	42,49,53,53	0
1	PCA	C	3	8/9	0.92	0.09	38,46,51,57	0
1	PCA	O	3	8/9	0.93	0.09	37,43,49,51	0
1	PCA	M	3	8/9	0.94	0.08	35,47,52,54	0
1	PCA	A	3	8/9	0.94	0.08	42,49,56,57	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

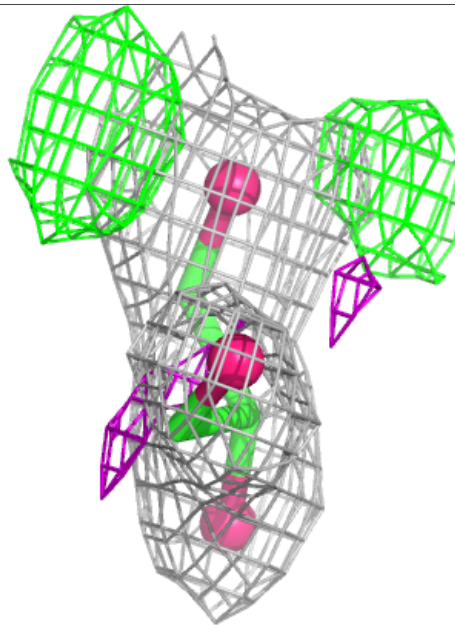
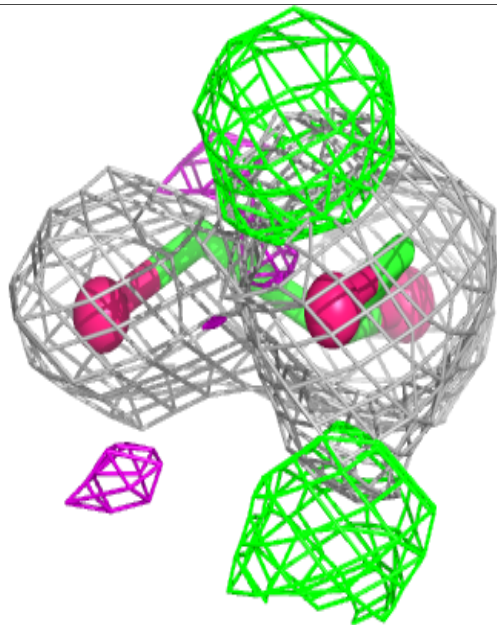
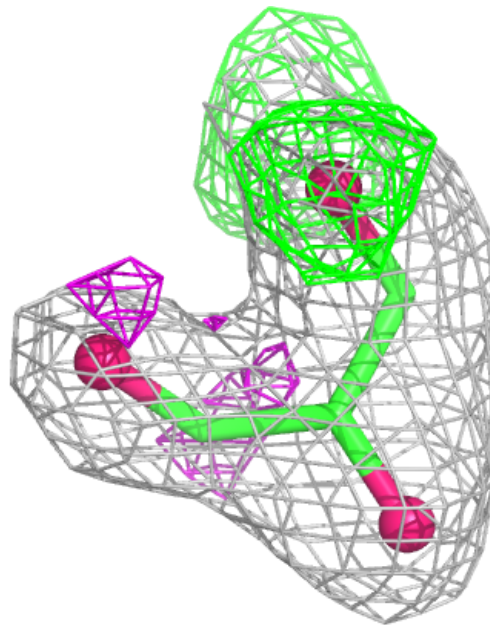
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	M	301	6/6	0.85	0.15	32,35,36,36	0
4	GOL	I	301	6/6	0.88	0.15	42,43,46,46	0
4	GOL	G	301	6/6	0.88	0.13	39,41,42,43	0
4	GOL	C	301	6/6	0.90	0.13	25,28,28,32	0
4	GOL	O	301	6/6	0.90	0.12	27,29,31,35	0
4	GOL	G	302	6/6	0.91	0.14	39,43,46,49	0
4	GOL	A	301	6/6	0.91	0.12	36,39,40,41	0
4	GOL	G	303	6/6	0.93	0.10	45,51,53,56	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

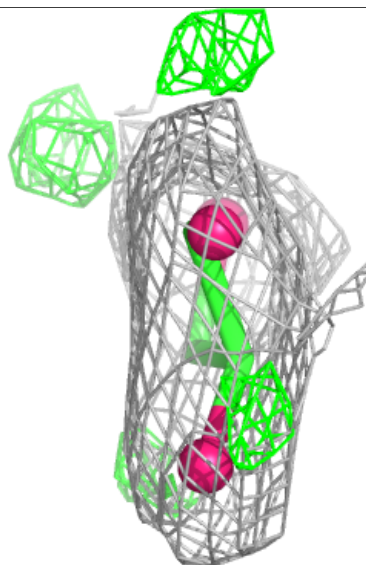
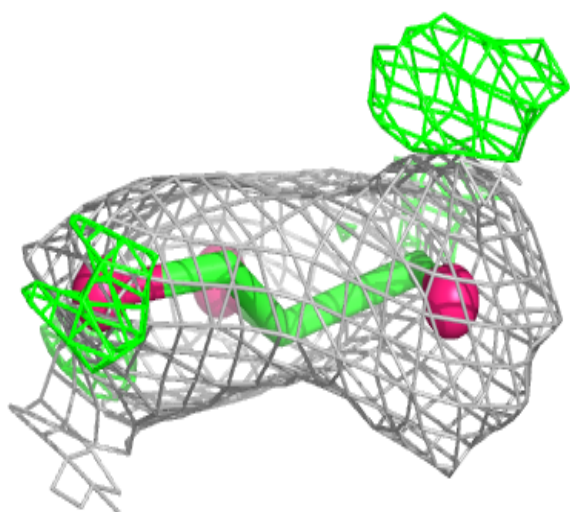
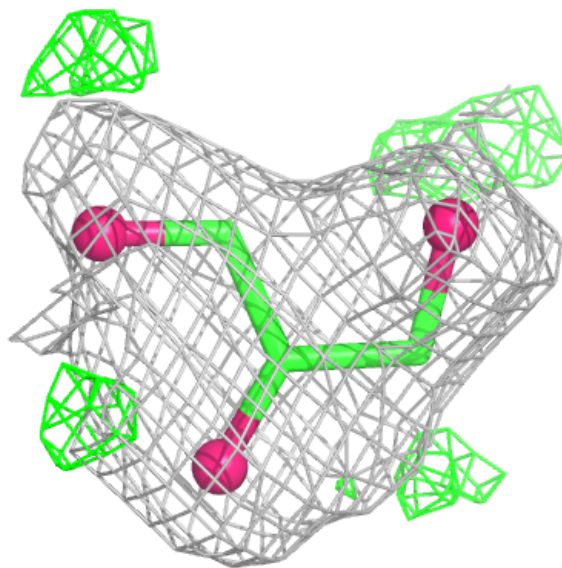
Electron density around GOL M 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



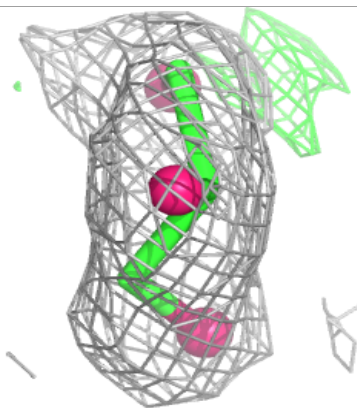
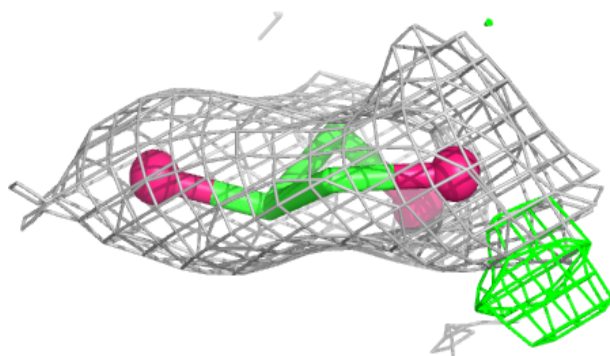
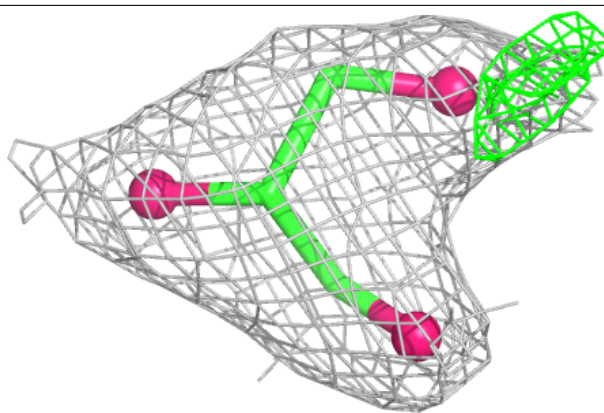
Electron density around GOL I 301:

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and green (positive)



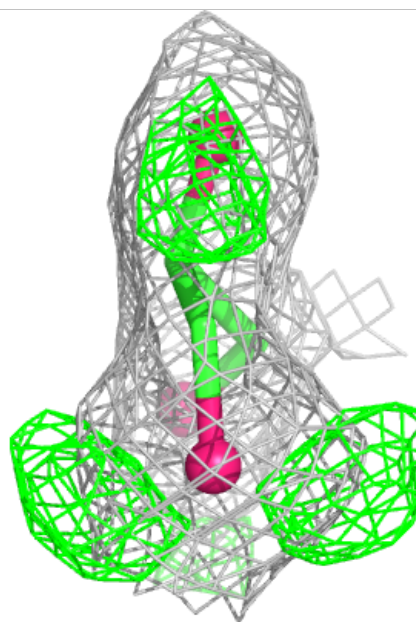
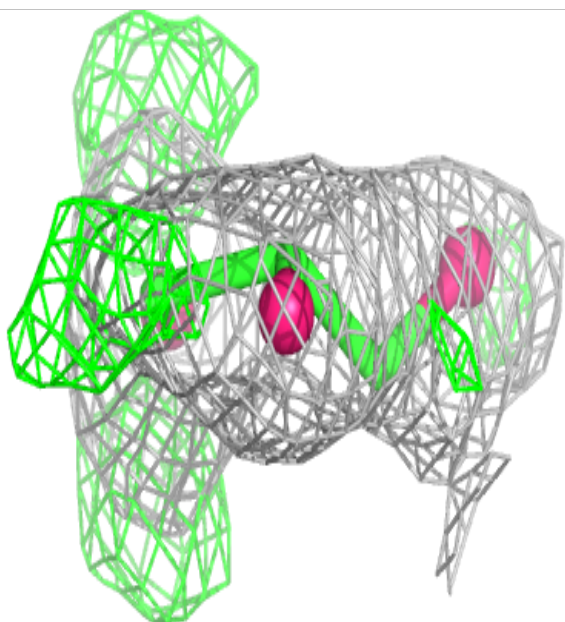
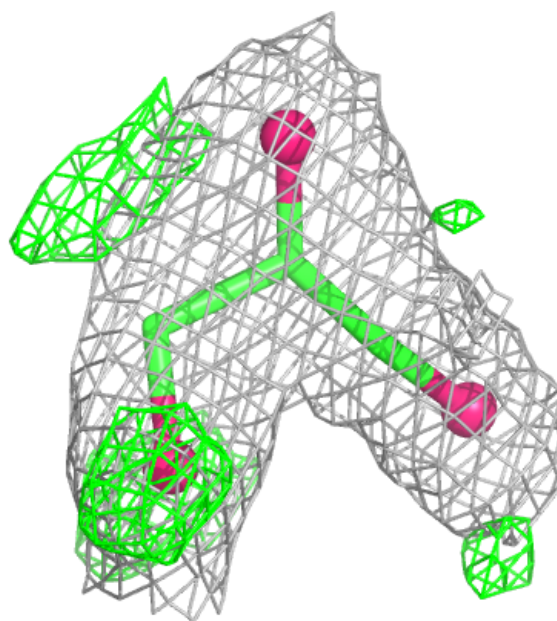
Electron density around GOL G 301:

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and green (positive)



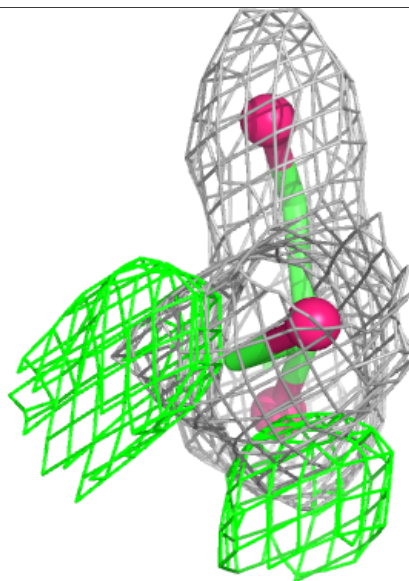
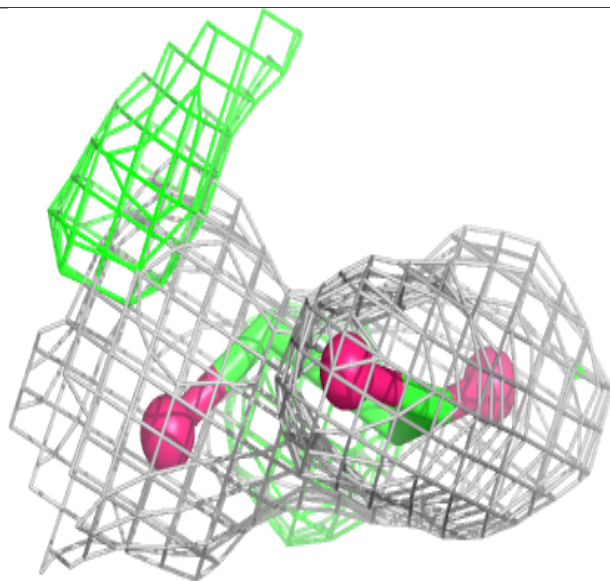
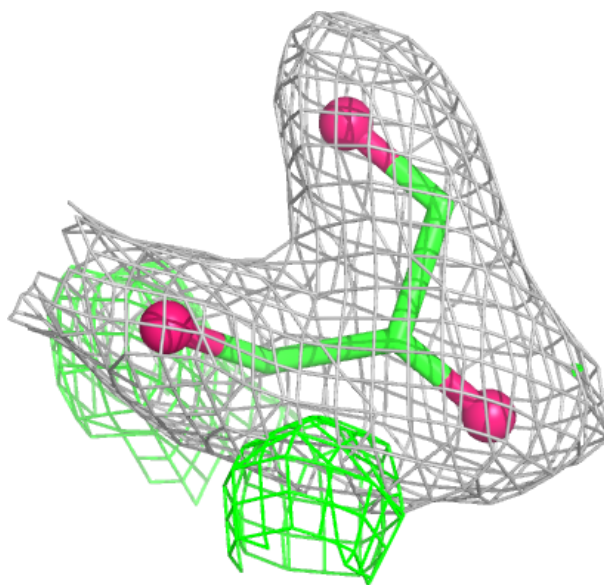
Electron density around GOL C 301:

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and green (positive)



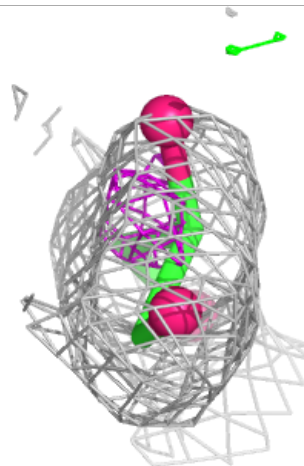
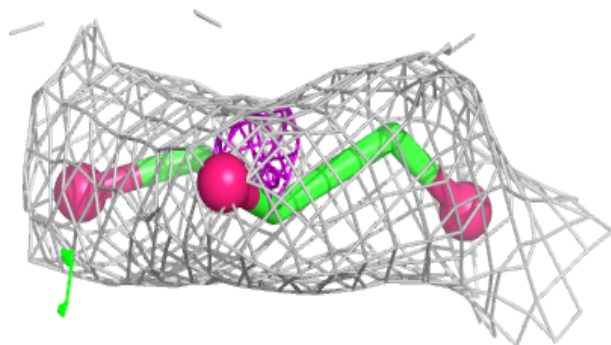
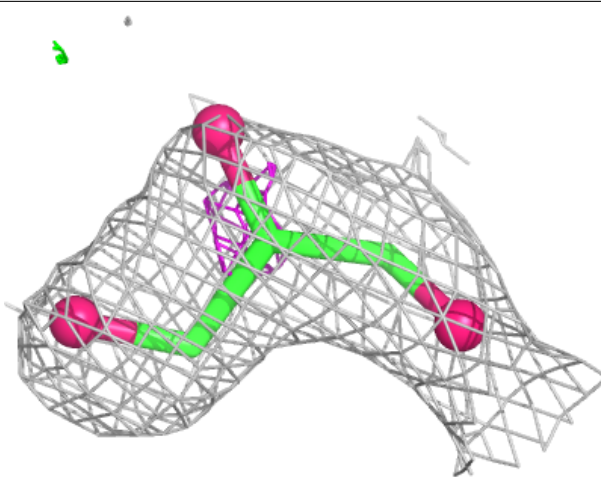
Electron density around GOL O 301:

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and green (positive)



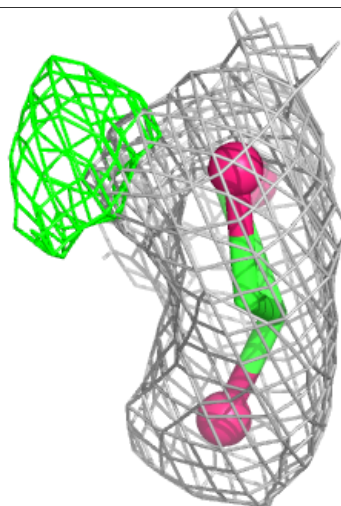
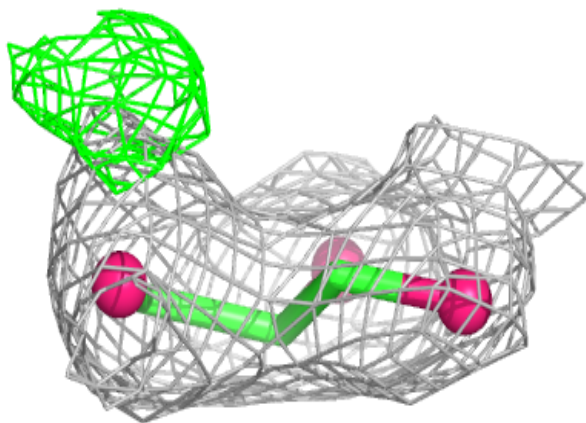
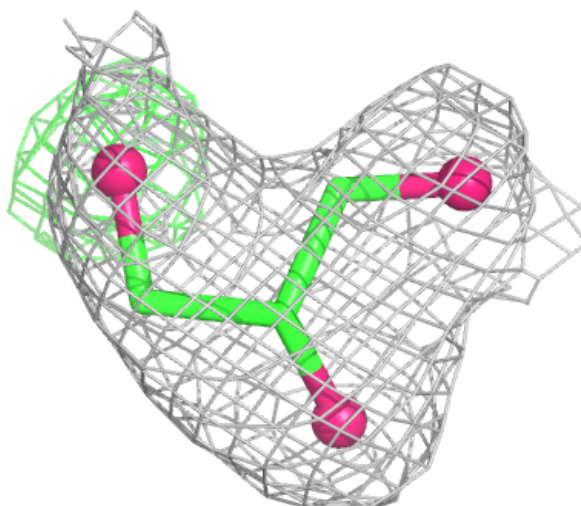
Electron density around GOL G 302:

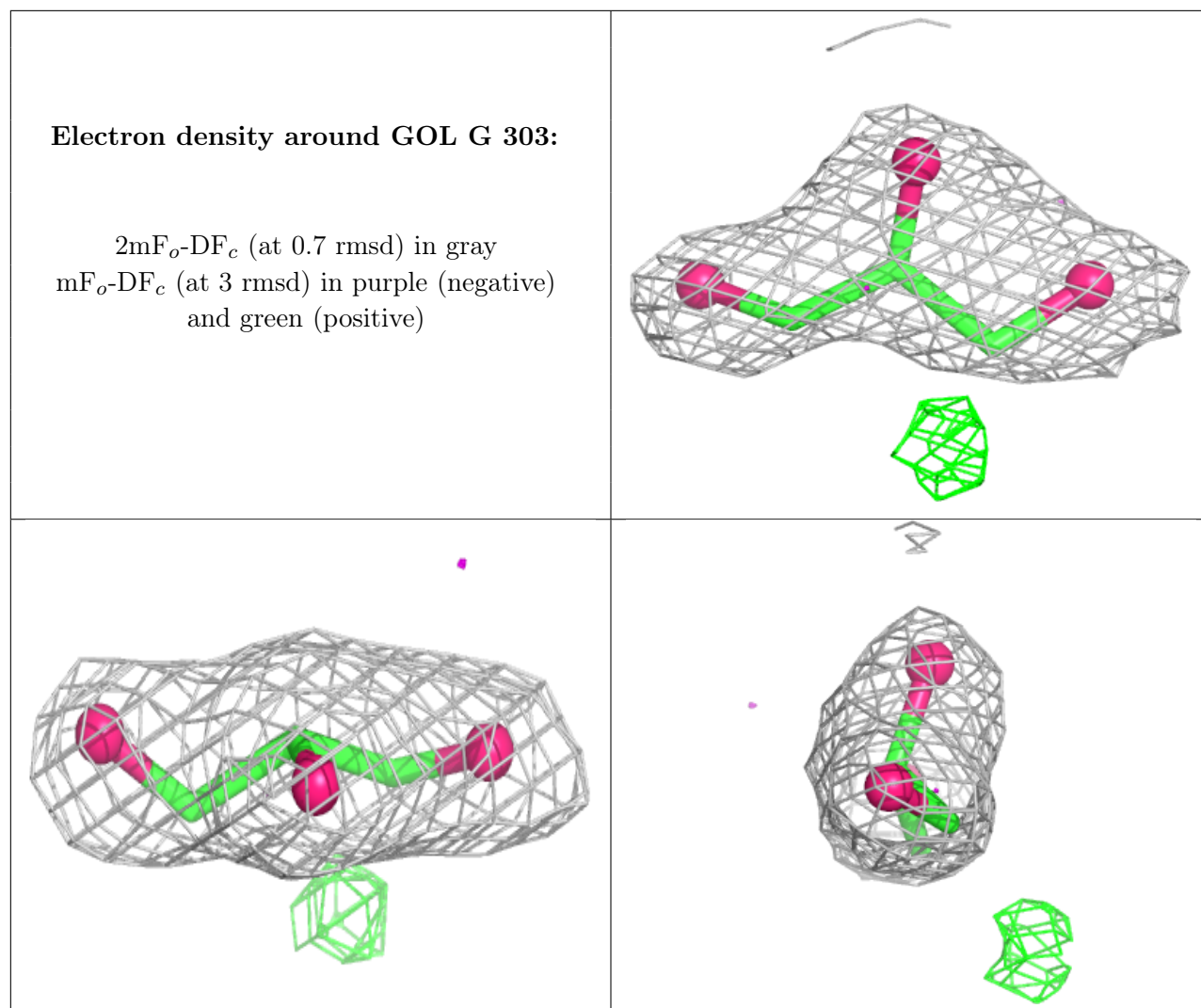
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GOL A 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.